

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110425\
 Data File : VX048478.D
 Acq On : 04 Nov 2025 13:00
 Operator : JC/MD
 Sample : Q3488-02 10X
 Misc : 3.75g/10mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MOO-25-0299

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
 Title : SW846 8260

Signal : TIC: VX048478.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.374	203	211	220	rBV	24882	49506	2.81%	0.659%
2	5.367	689	702	713	rBV3	63121	205949	11.67%	2.740%
3	5.532	713	729	754	rVB4	113669	525788	29.80%	6.995%
4	5.806	763	774	786	rBV2	42338	136361	7.73%	1.814%
5	5.934	786	795	814	rVB2	75847	227870	12.92%	3.032%
6	6.166	822	833	842	rBV7	5394	20954	1.19%	0.279%
7	6.592	893	903	918	rBV	37973	102871	5.83%	1.369%
8	6.739	918	927	946	rBV	217385	569341	32.27%	7.574%
9	7.354	1020	1028	1040	rVB6	9039	24946	1.41%	0.332%
10	8.629	1219	1237	1243	rBV	454966	808308	45.82%	10.753%
11	8.702	1243	1249	1274	rVB	1057023	1764114	100.00%	23.469%
12	10.037	1463	1468	1484	rVB	479938	688882	39.05%	9.165%
13	10.281	1500	1508	1514	rBV2	17706	33472	1.90%	0.445%
14	10.342	1514	1518	1529	rVB	16640	24551	1.39%	0.327%
15	11.061	1631	1636	1648	rVB	507108	701853	39.79%	9.337%
16	11.171	1648	1654	1664	rVB4	9779	21042	1.19%	0.280%
17	11.366	1680	1686	1691	rVV2	19000	39057	2.21%	0.520%
18	11.433	1691	1697	1699	rVV2	20241	38192	2.16%	0.508%
19	11.457	1699	1701	1706	rVB	41997	50082	2.84%	0.666%
20	11.549	1711	1716	1721	rBV	52867	72902	4.13%	0.970%
21	11.598	1721	1724	1731	rVB3	10139	17837	1.01%	0.237%
22	11.732	1743	1746	1755	rVB	31148	47525	2.69%	0.632%
23	11.872	1764	1769	1774	rVB	15772	22910	1.30%	0.305%
24	12.006	1785	1791	1797	rVV	528560	713764	40.46%	9.496%
25	12.067	1797	1801	1808	rVB3	9916	23788	1.35%	0.316%
26	12.311	1835	1841	1846	rVB4	22331	47567	2.70%	0.633%
27	12.402	1846	1856	1860	rBV	40276	56440	3.20%	0.751%
28	12.957	1940	1947	1952	rVB5	14057	32723	1.85%	0.435%
29	13.024	1952	1958	1961	rBV4	11757	18442	1.05%	0.245%
30	13.146	1971	1978	1982	rBV6	16417	31407	1.78%	0.418%
31	13.250	1992	1995	1996	rVV	32502	37611	2.13%	0.500%
32	13.274	1996	1999	2004	rVB3	40761	59931	3.40%	0.797%
33	13.402	2016	2020	2029	rVB3	28470	51992	2.95%	0.692%
34	13.567	2043	2047	2051	rBV5	19358	28091	1.59%	0.374%
35	13.835	2085	2091	2097	rVB5	16672	32530	1.84%	0.433%
36	13.908	2097	2103	2107	rBV6	13918	30000	1.70%	0.399%

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37	14.207	2146	2152	2159	rBV3	26862	45062	2.55%	0.599%
38	14.457	2189	2193	2202	rVB7	12471	25500	1.45%	0.339%
39	14.597	2212	2216	2218	rBV3	18480	26589	1.51%	0.354%
40	15.048	2286	2290	2298	rVB3	10630	20775	1.18%	0.276%
41	15.536	2364	2370	2375	rBV2	27951	40178	2.28%	0.535%

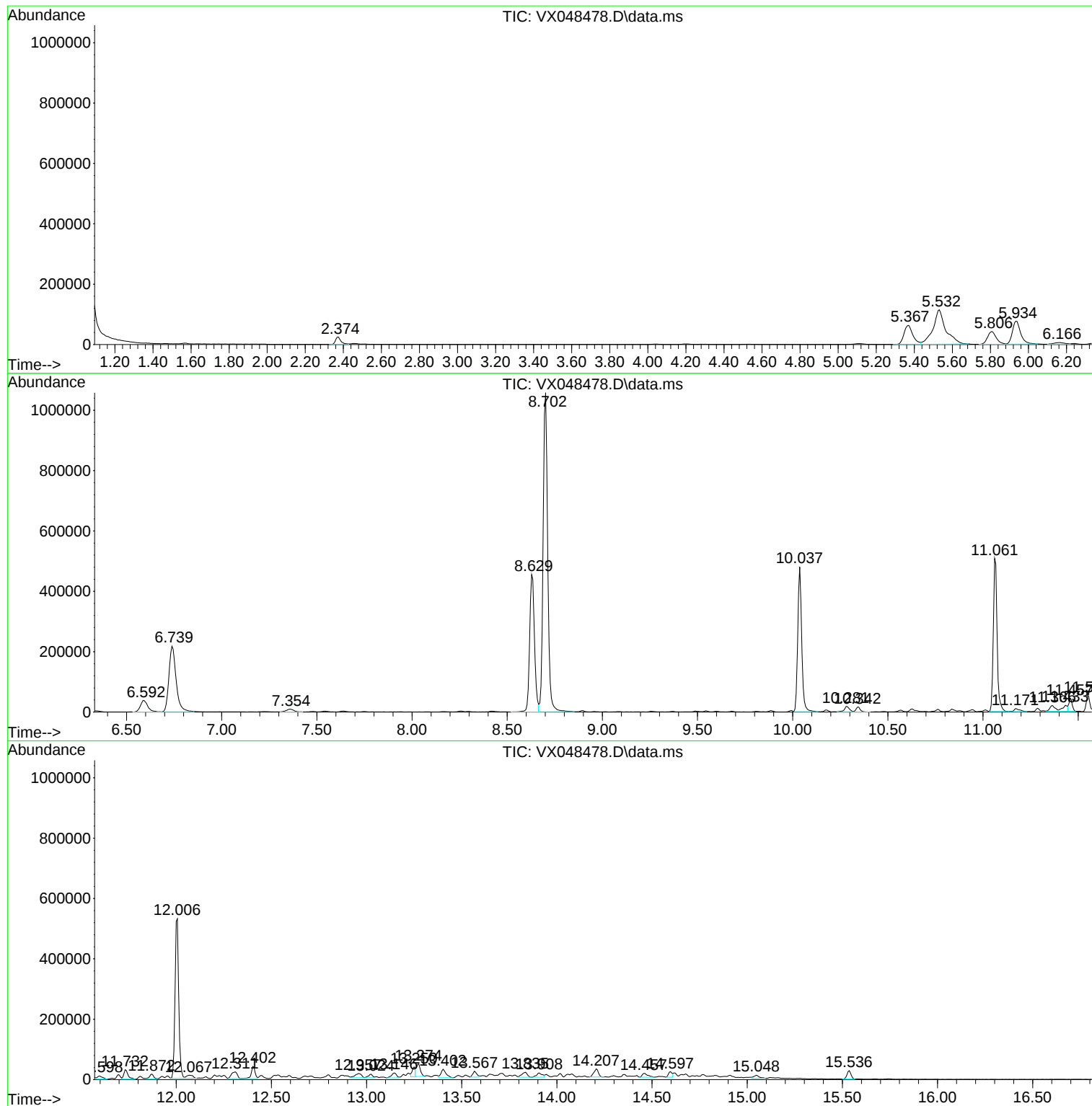
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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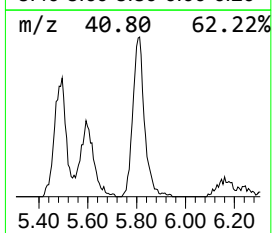
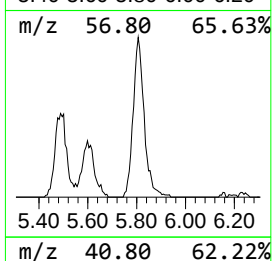
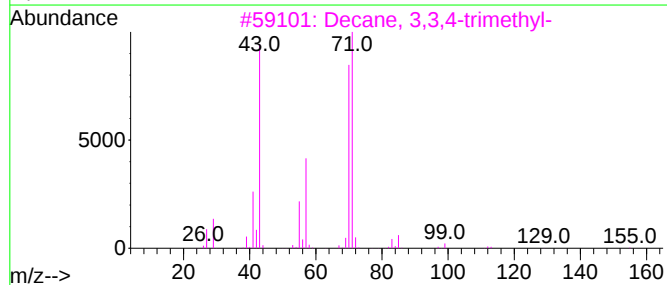
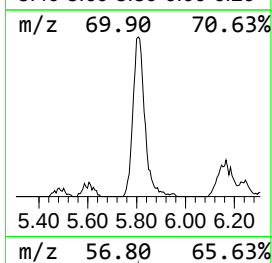
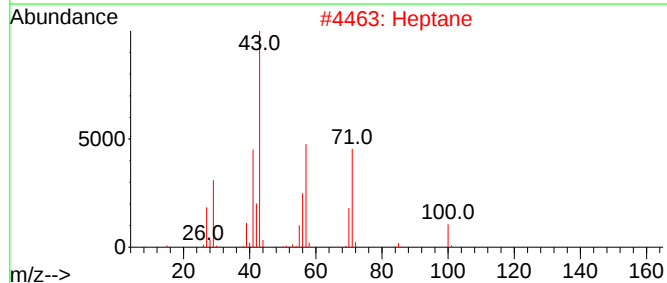
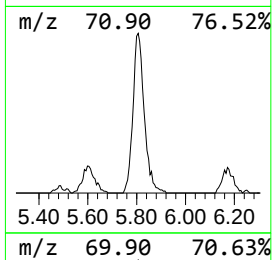
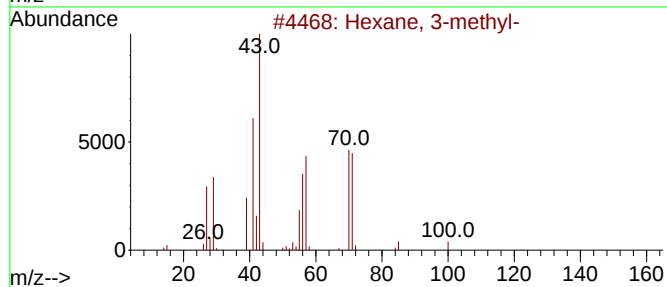
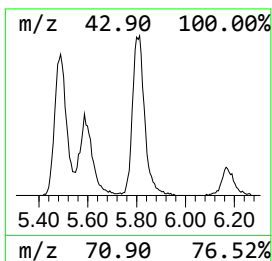
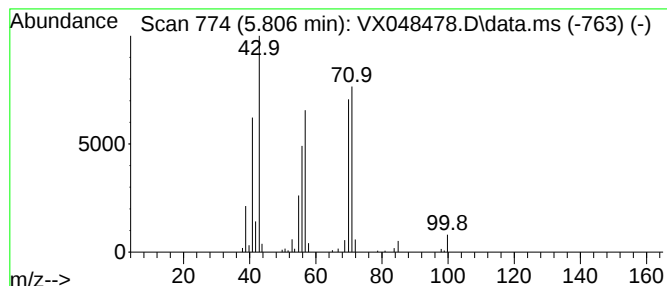
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102925W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.806	12.97 ug/l	136361	Pentafluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	90
2			Heptane	100	C7H16	000142-82-5	80
3			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	59



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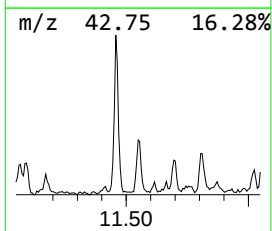
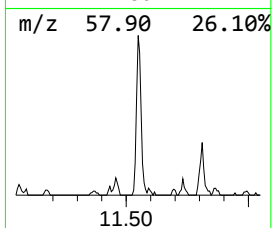
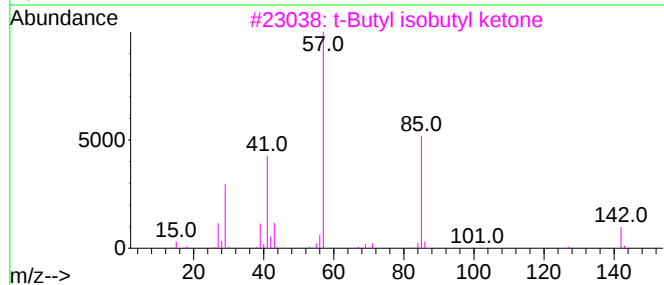
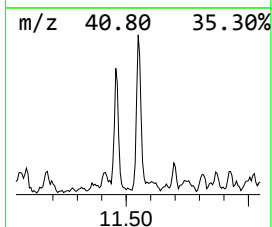
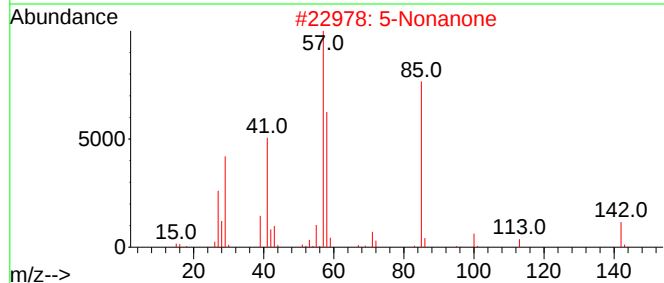
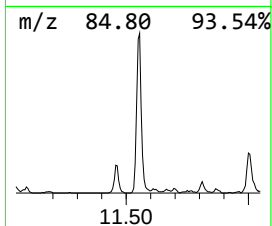
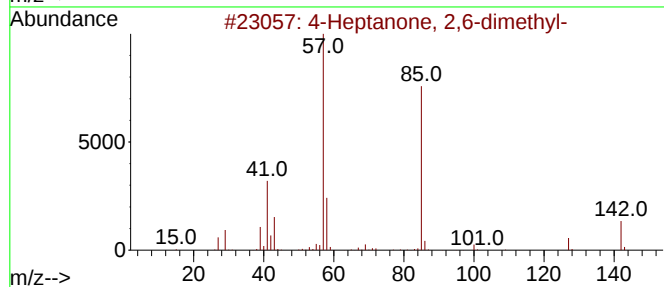
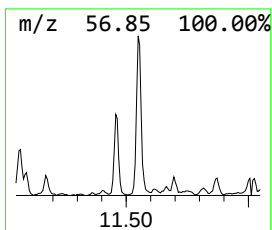
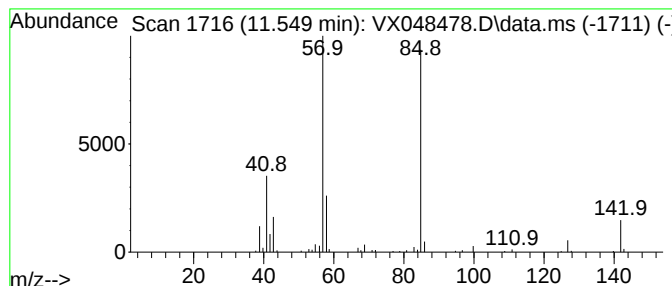
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Peak Number 3 4-Heptanone, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.549	5.11 ug/l	72902	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2			5-Nonanone	142	C9H18O	000502-56-7	59
3			t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
4			1-Propoxypropan-2-yl 2-methylbut...	202	C11H22O3	1000367-10-7	56
5			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	50



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	5.806	13.0	ug/l	136361	1	5.532	525788	50.0
4-Heptanone, 2,...	11.549	5.1	ug/l	72902	4	12.006	713764	50.0